Magnetic frustration in odd-membered $s = 3/2$ spin rings with bond defect

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9.7 cm

Chromium based rings are a family of molecular magnets which has been recently enlarged by a nine-membered frustrated homometallic ring (Cr_9). Many members of this family are considered for quantum computation and as a material for efficient storage devices.
In this presentation frustration effects in models of hypothetical and existing odd-membered antiferromagnetic chromium ($s = 3/2$) rings with a bond defect are studied by means of two numerical techniques: quantum transfer matrix and exact diagonalization. In order to identify a frustrated phase we calculate the full energy spectrum of the models and a number of thermodynamic quantities at low temperature. It is shown that total and local magnetizations, nearest-neighbor spin correlations and spin fluctuations can serve as consistent frustration signatures. Magnetizations and spin-spin correlations are reduced in the frustrated phase whereas fluctuations and correlations of fluctuations increase. We also determine the dependence of the critical value of the bond defect, at which a transition to the frustrated phase takes place, on the size of the system and external magnetic field. In the systems studied bipartiteness is not opposite to frustration as there are regions in the parameter space in which the system is neither bipartite nor frustrated.

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